IOP Conf. Series: Journal of Physics: Conf. Series **899** (2017) 092005 doi:10.1088/1742-6596/899/9/092005

Validation of the thermal NOx emissions model from a gas fuel combustor under atmospheric pressure

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Abstract: A description of various experimental and numerical investigation on NO_X emissions during the gas fuels combustion is presented. The selection of the validation object is justified. The NO_X formation and decomposition mechanisms are analyzed. The assembly of thermal NO_X formation and decomposition mechanisms was selected. Validation of the thermal NO_X emissions model by CFD-simulation was carried out. Validation is based on comparison of the numerical simulation results with well-known experimental data. The results of numerical simulation are analyzed. A method for improving the NO_X emissions computation from the gas fuel combustor is proposed.

1. Introduction

Currently, one of the most promising (for efficiency and environmental indicators) power generating system are integrated gasification combined cycles (IGCC). Approximately 2/3 of the IGCC output is production by the gas turbine, the remainder by steam-power cycle. The gas turbine fuel in IGCC is synthesis gas (syngas) produced by fossil fuel oxygen- or air-blown gasification (lower heating value (LHV) – 4 to 13 MJ/m^3 at 273 K, 1 atm) [1]. During the syngas combustion technologies development the much attention is paid to the environmental indicators of IGCC combustor, namely to nitrogen oxides (NOx) emissions.

The results of experimental investigation of NO_X emissions during the various gas fuels combustion are presented in [2, 3, 4]. Hasegawa et al. [2] experimentally evaluated the effect of nitrogen dilution of oxidant and gas fuel (a mixture of CO and H_2) on the rate of thermal and fuel NO_X emissions of two-stage combustor with diffusion burner. Experiments have shown that dilution significantly reduces the thermal NO_X emissions over a wide range of the equivalence ratio in the primary combustion zone (φ_p) and slightly affects the fuel NO_X emissions in the range φ_p>1. Feng et al. [3] shows the effect of the CO_2 content on the NO_X decomposition rate in methane combustion. Experiments have shown that the presence of CO_2 has little effect on the NO_X decomposition. Liu et al. [4] investigated the catalytic reduction of NO_X emissions due to injection of hydrazine hydrate into the hot exhaust gases. Authors identifies two temperature ranges of exhaust gases for effective denitrification: 820-960 K and 1260-1330 K.

At present, a CFD-methods are well established for investigation of IGCC combustors behavior, but before the commencement of work it is expedient to verify the NO_X formation and decomposition mechanisms.

Numerical studies of NO_X formation and decomposition mechanisms have been carried out in [5, 6, 7, 8]. Jurena et al. [5] numerically investigated the influence of the Magnussen constant of Eddy Dissipation combustion model on the gas combustion characteristics in diffusion burner. The investigation was carried out based on comparison of calculated results and experimental data. They showed that the optimal value of the Magnussen constant for predicting the gas combustion characteristics is 1.2. Goswami et al. [6], Volkov et al. [7] verified the thermal and fuel NO_X formation and decomposition mechanisms database. Bowman et al. [8] describes in detail the mechanisms of pollutant formation and decomposition during the gas combustion. Woo et al. [9] carried out the numerical and experimental studies of the fuel NO_X formation in the CH_4-NH_3 mixture combustion. The N_2/O_2 ratio in the oxidizer was varied in order to determine the regime of low-NO_X CH_4-NH_3 mixture combustion.

At present, in operating IGCC application the fossil fuel entrained-flow gasification technology and the cold gas cleanup (CGC) system for pollutant (fuel sulfur- (H_2S, COS) and nitrocompound (NH_3, HCN), mercury, dust, etc.) removed from syngas before combustion in gas turbine combustor. Fossil fuel entrained-flow gasification technologies provides the hydrocarbons (prompt NO_X sources) content in syngas does not exceed 2 vol.% [1]. CGC system provides fuel nitrocompounds (fuel NO_X sources) content in syngas <50 ppm [10]. Such negligible concentrations of hydrocarbons and fuel nitrocompounds in syngas provides to evaluate the IGCC combustor NO_X emissions by only thermal NO_X content in exhaust gases, without taking into account the prompt and fuel NOx availability.

In present work carried out the validation of the thermal NO_X emissions model (include the NO_X and other chemical compounds formation and decomposition mechanisms) in gas fuel combustor, which is similar in composition to the syngas of coal oxygen-blown gasification. Validation was carried out based on comparison of calculated results with well-known experimental data.

2. Method

Validation of the thermal NOx emissions model is based on a comparison of the calculated results (by Ansys CFX) and experimental data published by Hasegawa et al. [2]. According to Hasegawa et al. [2], in the experimental combustor (figure 1) organized two-stage supply of oxidizer (air). It organized to simulate the industrial gas turbine combustor operating conditions, namely to achieve the required flame length and temperature distribution in the longitudinal section of the combustor.

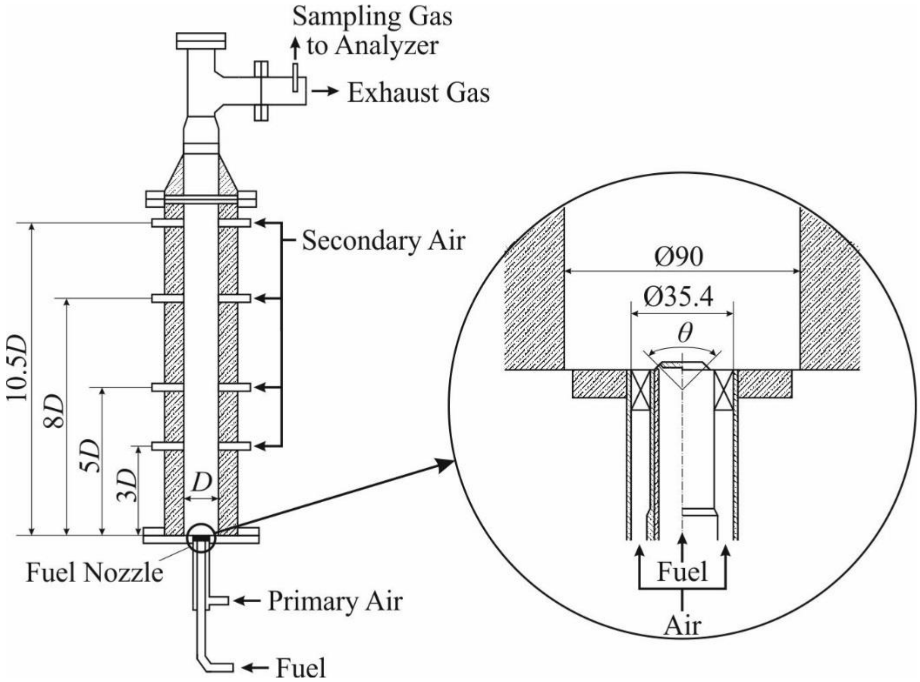

Figure 1. Scheme of experimental combustor [2].

Hasegawa et al [2] considered the influence of the equivalence ratio in the primary combustion zone (φ_p) of the experimental combustor on the thermal NOx emissions. In the experiments, the temperature of the exhaust gases was maintained at ~1500°C. The gas fuel flow rate and composition, the total air flow rate (the sum of the primary and secondary air) and the temperature of the reacting agent were unchanged. Gas fuel is a H_2-CO mixture with a ratio of H_2/CO=30/70 vol.%/vol.% («model syngas» of coal oxygen-blown gasification).

A CFD-model of the experimental combustor (figure 1) is created to the numerical simulation and the following parameters was set:

1) combustion model – Eddy Dissipation, adjusted by Jurena et al. [5];
2) turbulence model – Shear Stress Transport, based on work of Menter [11];
3) thermal radiation model – Monte Carlo;
4) combustion mechanisms – standard mechanisms of H_2 and CO combustion in terms of the radicals;
5) thermal NOx formation and decomposition mechanisms – adopted from Goswami et al. [6] (reactions №25-28 and 101). In numerical simulation, thermal NOx emissions were evaluated by calculated NO content in exhaust gases. Because NO content in exhaust gases during the gas fuel combustion is about 90% of all NOx [8].

The parameters of the reacting agents are setting according to the experiment [2]. The temperature of the exhaust gases was maintained at 1500±20°C. The equivalence ratio φ_p was varied in the range 0.5 to 2. The mass flow rate of gas fuel was set according to the experiment, the mass flow rates of primary and secondary air were determined by equations (1) and (2).

$$\varphi_p = \frac{\left(\dfrac{M_F}{M_{PA}}\right)^{act}}{\left(\dfrac{M_F}{M_A}\right)^{st}} \tag{1}$$

$$M_T = M_{PA} + M_{SA} \tag{2}$$

where M_F, M_{PA}, M_{SA}, M_T, M_A, – mass flow rates of gas fuel, primary air, secondary air, total air and stoichiometric air; $\left(\dfrac{M_F}{M_{PA}}\right)^{act}$ – actual fuel-air ratio in the primary combustion zone of experimental combustor; $\left(\dfrac{M_F}{M_A}\right)^{st}$ – stoichiometric fuel-air ratio in the primary combustion zone of experimental combustor.

3. Results

Because NO content in exhaust gases during the syngas combustion is about 90% of all NOx [8], the thermal NOx emissions were evaluated by calculated NO content in exhaust gases.

A comparison of calculated results and experimental data on NOx emissions depending on φ_p is presented in table 1.

Table 1. Comparison of calculated results and experimental data.

Equivalence ratio in the primary combustion zone (φ_p)		0.62	1	1.5	2
Excess air coefficient in the primary combustion zone (α_p)		1.6	1	0.7	0.5
$NOx_{th}(16\%O_2)$, ppm	Hasegawa et al. [2]	36	97.2	19	14
	Present work	41	118	35	16.8
Spread of computational results from experimental data, %		12	18	46	17

A visual comparison of the calculated results (predicted curve) and the experimental data [2] is shown in figure 2.

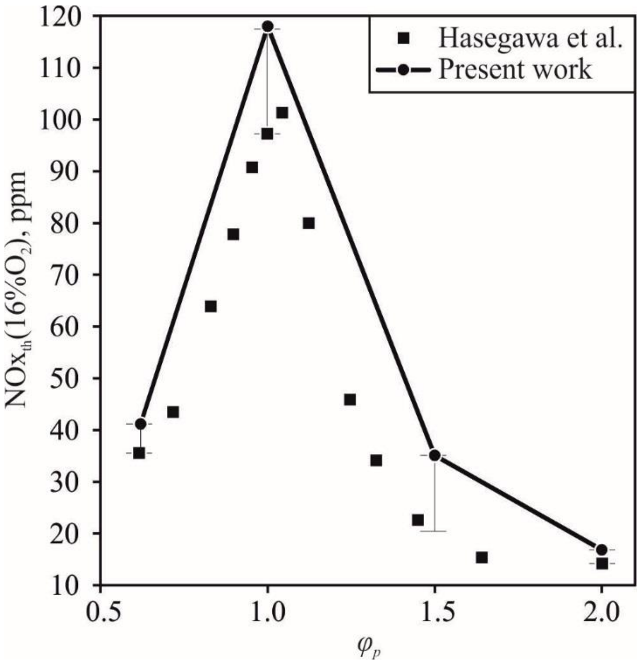

Figure 2. Comparison of the predicted curve and the experimental data [2].

The total RMS deviation of CFD-simulation was 0.15. The deviation of the predicted curve from the experimental data is observed in all points. Probably, the deviation is due to the CFD solver RMS deviation at prediction the flame maximum temperature coupled with the inaccuracy in determining and controlling the exhaust gases temperature or φ_p in the experiment.

4. Conclusions

Numerical simulation showed that the total RMS deviation in CFD prediction is 0.15. Generally, it is seen that the predicted curve of the combustor NO_X emissions is closely spaced to the experimental data. That indicates the possibility of further use of the developed CFD-model for the prediction of NO_X emissions from combustors of IGCC with CGC systems. For the prediction of NO_X emissions from combustors of IGCC with warm (WGC) or hot gas (HGC) cleanup systems, it is advisable to validation the fuel NO_X emissions model. Because in the IGCC with WGC or HGC systems the fuel nitrocompounds content in syngas before the gas turbine combustor can reach up to 1000-3000 ppm.
The selected assembly allows to predict NO_X emissions with satisfactory accuracy. In case of necessary to improve the accuracy of results, it is recommended to use a more detailed chemistry in terms of the effect of the NO_2, N_2O, etc. formation and decomposition on total NO_X emission from gas turbine combustor.

Acknowledgments

The reported study has been supported by RFBR, research project No. 16-38-00479

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